Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

pH-metric Result

logP (XH +)	0.77	±0.03 (n=50)
logP (neutral X)	3.95	±0.02 (n=50)
RMSD	0.422	

18C-24004 Points 1 to 23

M04_octanol concentration factor	0.620
Carbonate	0.0570 mM
Acidity error	0.07992 mM

18C-24004 Points 24 to 50

M04_octanol concentration factor	0.641
Carbonate	0.1306 mM
Acidity error	-0.26645 mM

18C-24004 Points 51 to 77

M04_octanol concentration factor	0.822
Carbonate	0.1176 mM
Acidity error	-0.01548 mM

Warnings and errors

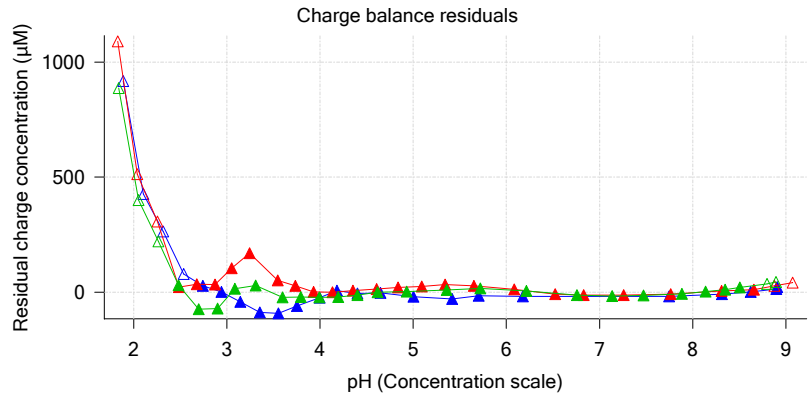
Errors	None
Warnings	None

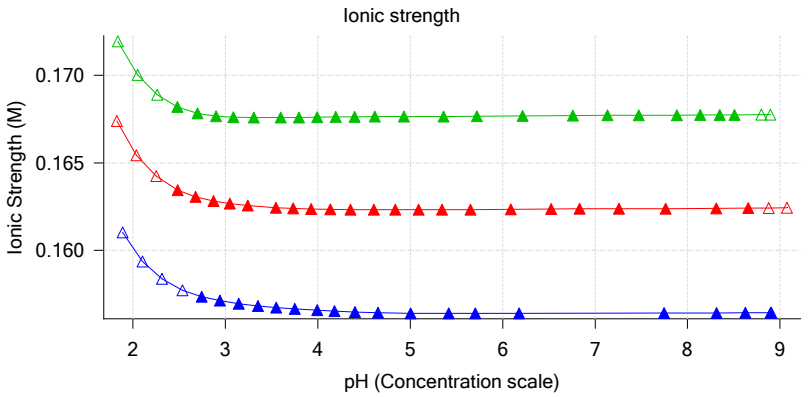
Sample logD and percent species

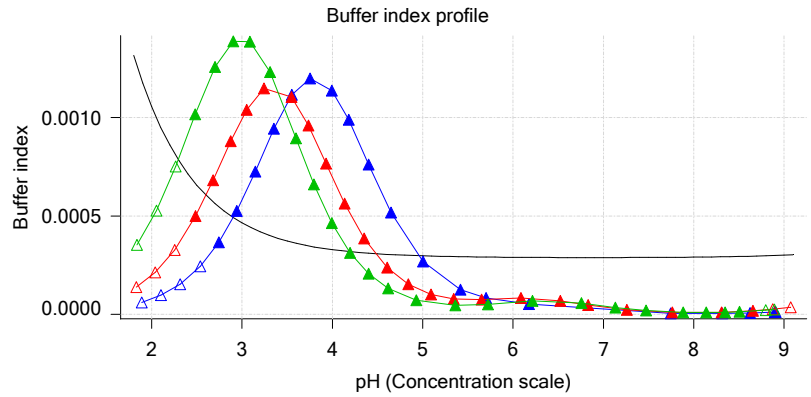
pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanol	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.78	14.18 %	0.00 %	84.45 %	1.37 %	
1.200	0.79	14.07 %	0.00 %	83.78 %	2.15 %	Stomach pH
2.000	0.84	12.63 %	0.00 %	75.19 %	12.18 %	
3.000	1.19	6.03 %	0.01 %	35.87 %	58.10 %	
4.000	2.01	0.97 %	0.01 %	5.76 %	93.26 %	
5.000	2.94	0.10 %	0.01 %	0.61 %	99.27 %	
6.000	3.67	0.01 %	0.01 %	0.06 %	99.92 %	
6.500	3.84	0.00 %	0.01 %	0.02 %	99.97 %	
7.000	3.92	0.00 %	0.01 %	0.01 %	99.98 %	
7.400	3.94	0.00 %	0.01 %	0.00 %	99.99 %	Blood pH
8.000	3.95	0.00 %	0.01 %	0.00 %	99.99 %	
9.000	3.95	0.00 %	0.01 %	0.00 %	99.99 %	
10.000	3.95	0.00 %	0.01 %	0.00 %	99.99 %	
11.000	3.95	0.00 %	0.01 %	0.00 %	99.99 %	
12.000	3.95	0.00 %	0.01 %	0.00 %	99.99 %	

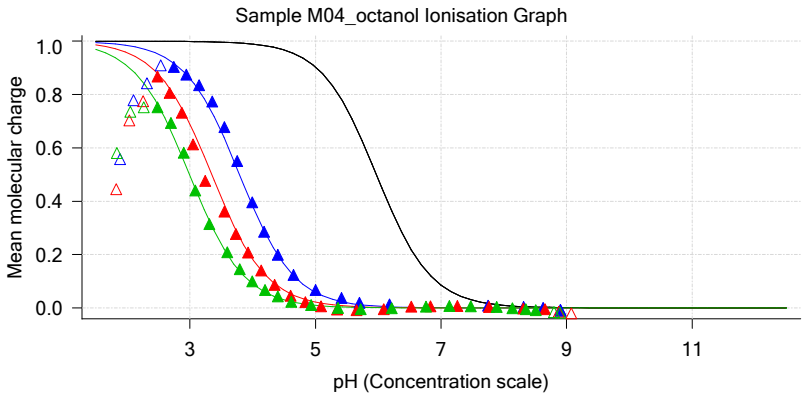
Sample name:	**M04_octanol**	Experiment start time:	**3/24/2018 4:11:23 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Dorothy Levorse**
Assay ID:	**18C-24004**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**		

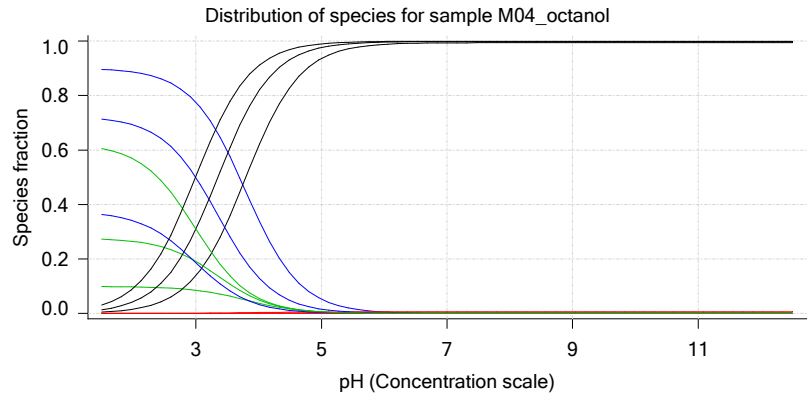
Graphs

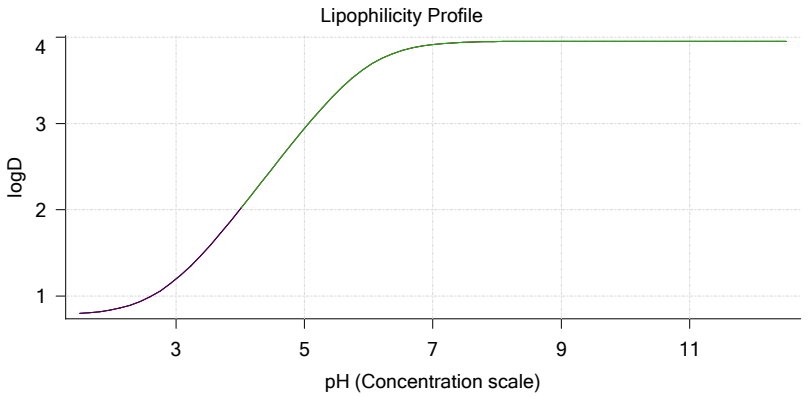


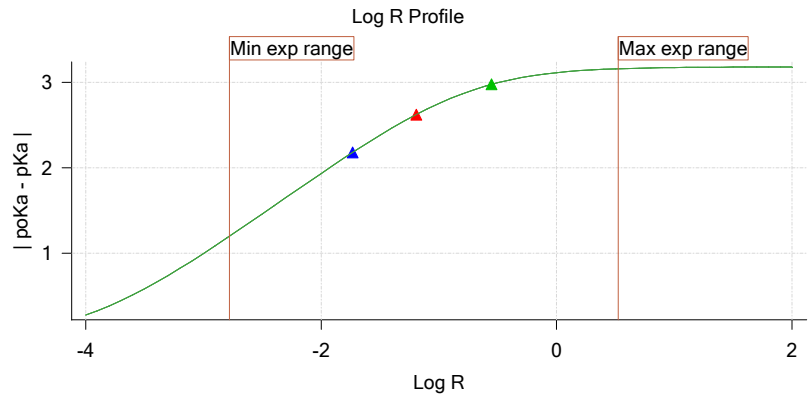


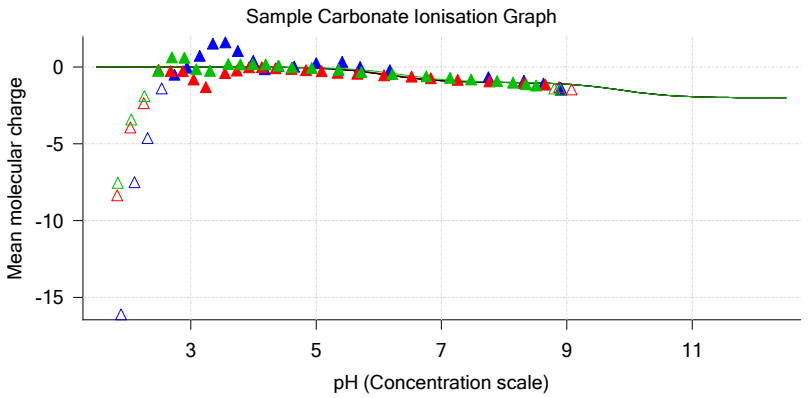








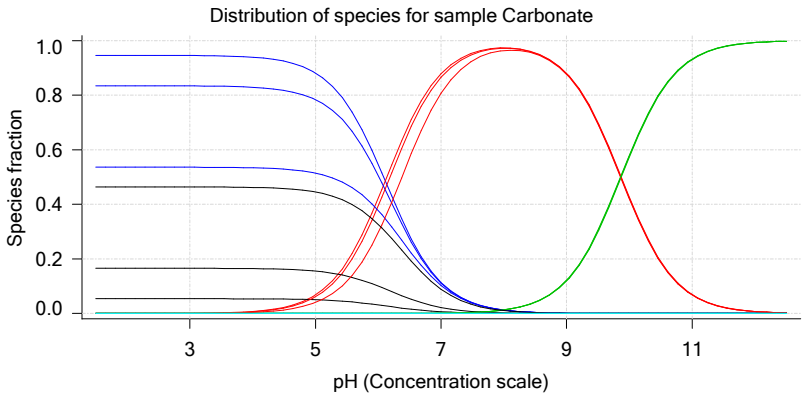




Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Graphs (continued)



Sample name:	**M04_octanol**	Experiment start time:	**3/24/2018 4:11:23 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Dorothy Levorse**
Assay ID:	**18C-24004**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 1 of 3 18C-24004 Points 1 to 23

Overall results

RMSD	0.635
Average ionic strength	0.157 M
Average temperature	24.9°C
Partition ratio	0.0185 : 1
Analyte concentration range	3292.8 µM to 3384.5 µM
Total points considered	19 of 23

Warnings and errors

Errors	None
Warnings	Sample concentration factor out of range

Four-Plus parameters

Alpha	0.119	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
S	0.9972	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
jH	0.9	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
jOH	-0.3	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r

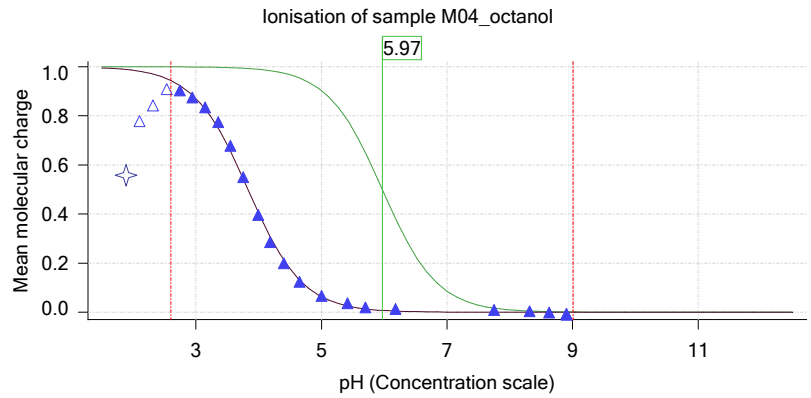
Titrants

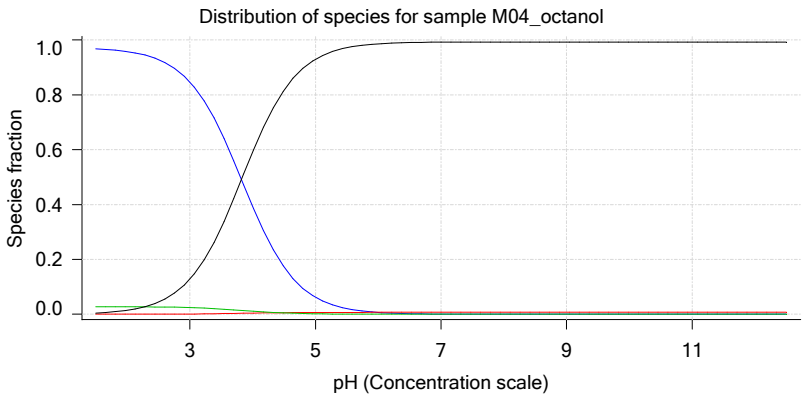
0.50 M HCl	0.997124	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
0.50 M KOH	1.003190	3/24/2018 4:11:23 AM	C:\Sirius_T3\KOH18C23.t3r

Sample

M04_octanol concentration factor	0.620
Base pKa 1	5.97
logP (XH +)	0.19
logP (neutral X)	3.88

Sample graphs

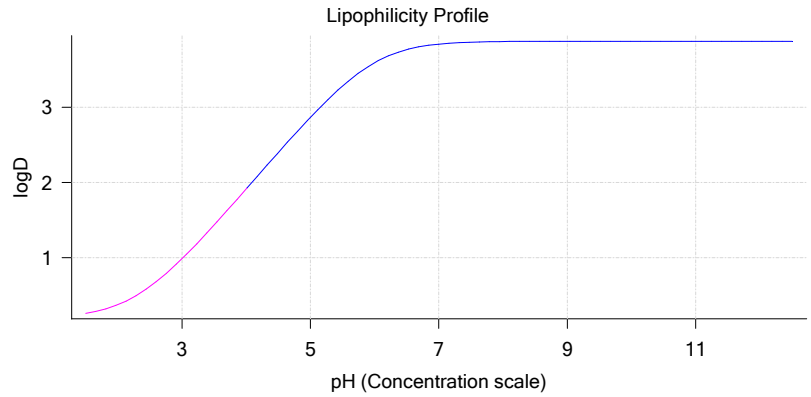




Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Sample graphs (continued)



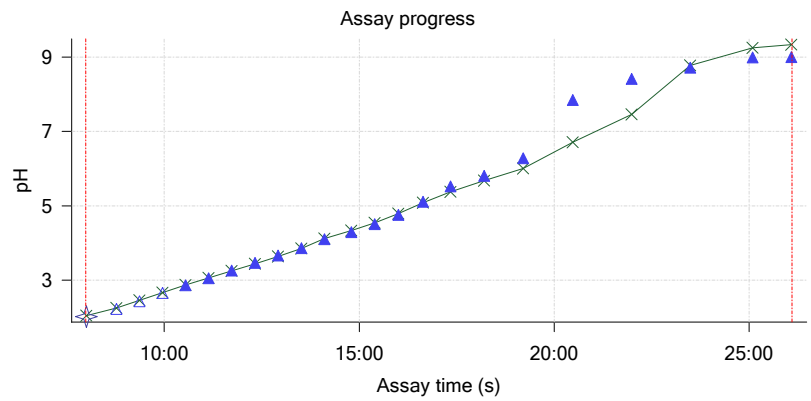
Sample logD and percent species

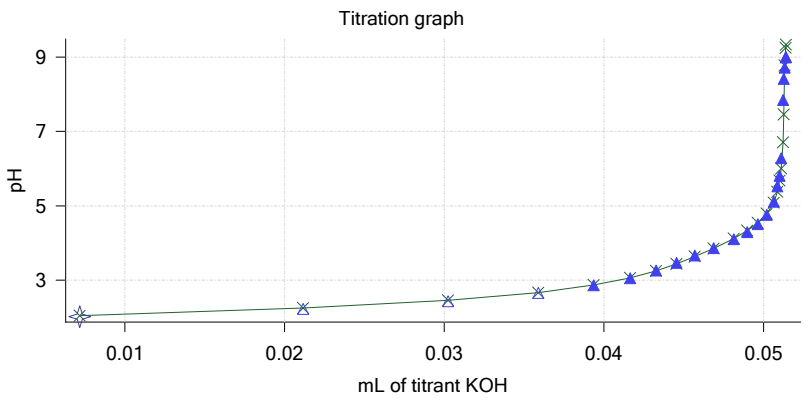
pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanol	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.21	97.07 %	0.00 %	2.78 %	0.15 %	
1.200	0.22	96.99 %	0.00 %	2.78 %	0.23 %	Stomach pH
2.000	0.37	95.80 %	0.01 %	2.74 %	1.44 %	
3.000	0.99	84.72 %	0.09 %	2.43 %	12.76 %	
4.000	1.91	39.28 %	0.42 %	1.13 %	59.18 %	
5.000	2.87	6.17 %	0.66 %	0.18 %	92.99 %	
6.000	3.59	0.65 %	0.70 %	0.02 %	98.63 %	
6.500	3.77	0.21 %	0.70 %	0.01 %	99.08 %	
7.000	3.84	0.07 %	0.71 %	0.00 %	99.23 %	
7.400	3.87	0.03 %	0.71 %	0.00 %	99.27 %	Blood pH
8.000	3.88	0.01 %	0.71 %	0.00 %	99.29 %	
9.000	3.88	0.00 %	0.71 %	0.00 %	99.29 %	
10.000	3.88	0.00 %	0.71 %	0.00 %	99.29 %	
11.000	3.88	0.00 %	0.71 %	0.00 %	99.29 %	
12.000	3.88	0.00 %	0.71 %	0.00 %	99.29 %	

Carbonate and acidity

Carbonate 0.057 mM
Acidity error 0.080 mM

Other graphs

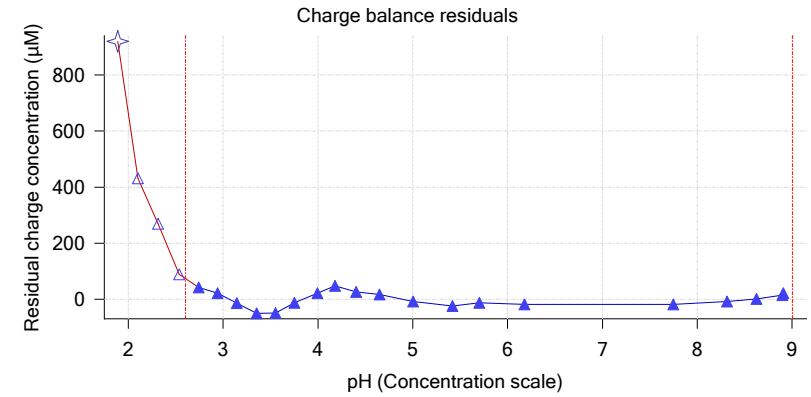


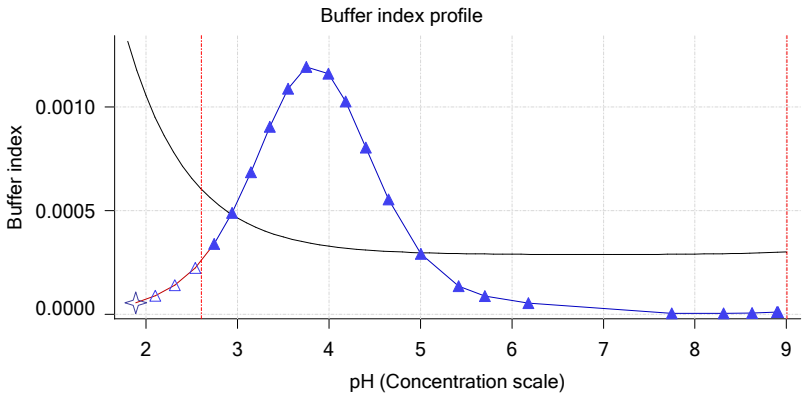


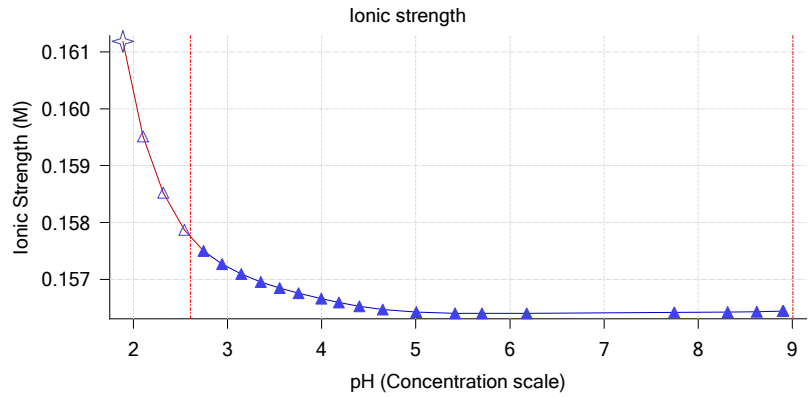
Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

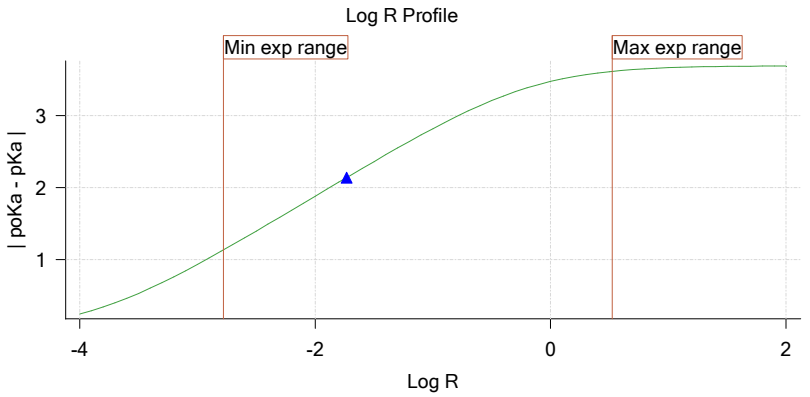
Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

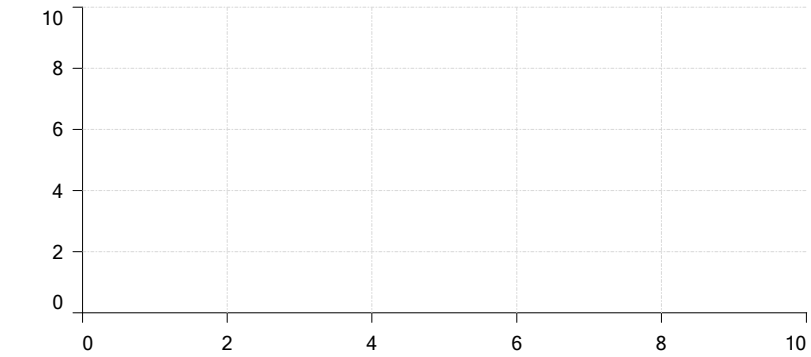
Other graphs (continued)

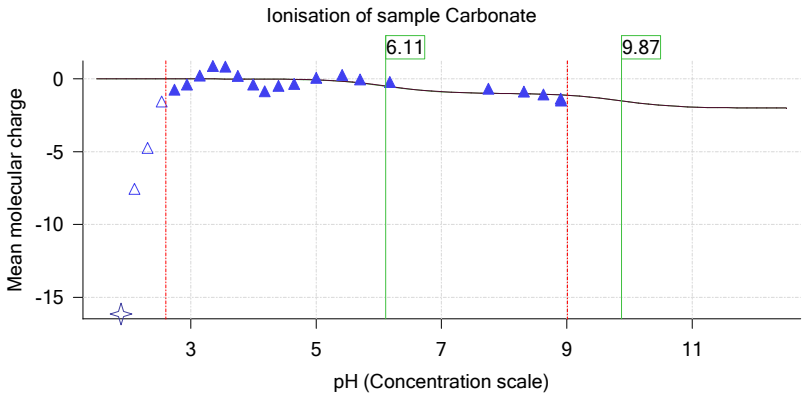












Sample name:	**M04_octanol**	Experiment start time:	**3/24/2018 4:11:23 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Dorothy Levorse**
Assay ID:	**18C-24004**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 2 of 3 18C-24004 Points 24 to 50

Overall results

RMSD	0.240
Average ionic strength	0.163 M
Average temperature	25.0°C
Partition ratio	0.0642 : 1
Analyte concentration range	2954.9 µM to 3043.2 µM
Total points considered	22 of 27

Warnings and errors

Errors	None
Warnings	Sample concentration factor out of range

Four-Plus parameters

Alpha	0.119	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
S	0.9972	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
jH	0.9	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
jOH	-0.3	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r

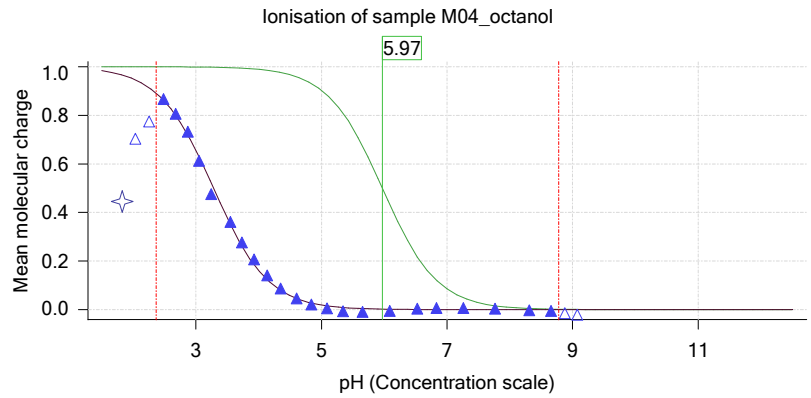
Titrants

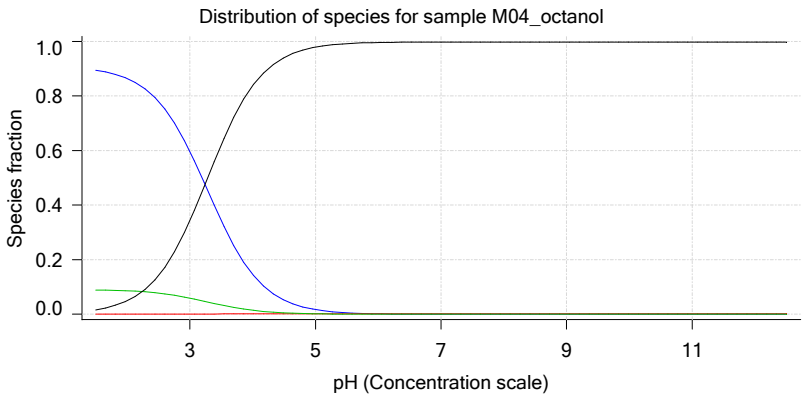
0.50 M HCl	0.997124	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
0.50 M KOH	1.003190	3/24/2018 4:11:23 AM	C:\Sirius_T3\KOH18C23.t3r

Sample

M04_octanol concentration factor	0.641
Base pKa 1	5.97
logP (XH +)	0.19
logP (neutral X)	3.92

Sample graphs

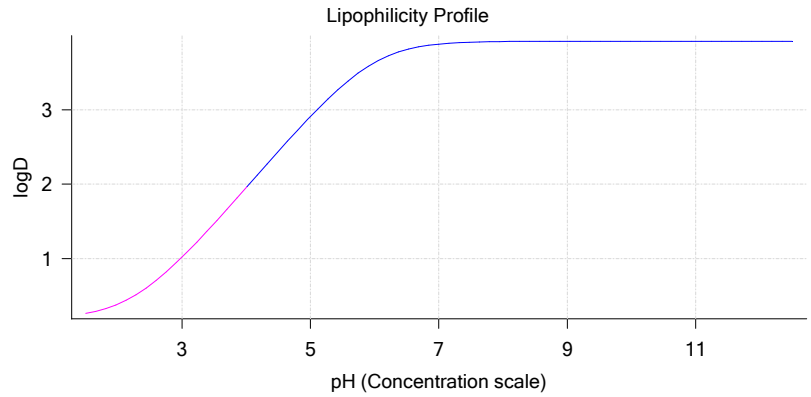




Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Sample graphs (continued)



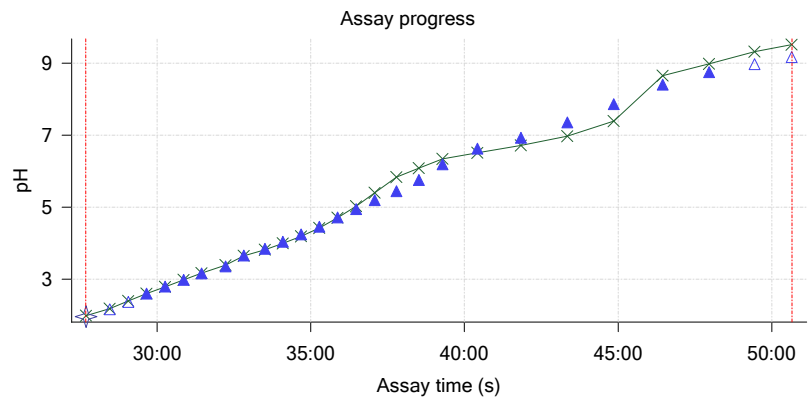
Sample logD and percent species

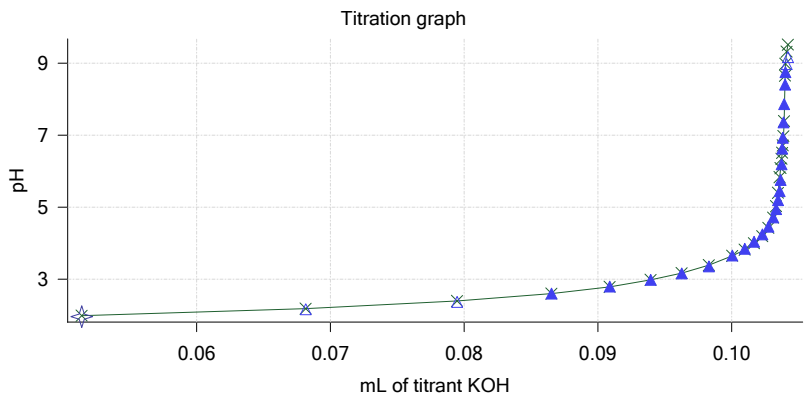
pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanol	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.21	90.48 %	0.00 %	9.00 %	0.52 %	
1.200	0.23	90.21 %	0.00 %	8.97 %	0.82 %	Stomach pH
2.000	0.39	86.44 %	0.01 %	8.60 %	4.96 %	
3.000	1.02	59.74 %	0.06 %	5.94 %	34.25 %	
4.000	1.95	14.61 %	0.16 %	1.45 %	83.78 %	
5.000	2.91	1.71 %	0.18 %	0.17 %	97.94 %	
6.000	3.63	0.17 %	0.19 %	0.02 %	99.62 %	
6.500	3.81	0.06 %	0.19 %	0.01 %	99.75 %	
7.000	3.88	0.02 %	0.19 %	0.00 %	99.79 %	
7.400	3.90	0.01 %	0.19 %	0.00 %	99.81 %	Blood pH
8.000	3.92	0.00 %	0.19 %	0.00 %	99.81 %	
9.000	3.92	0.00 %	0.19 %	0.00 %	99.81 %	
10.000	3.92	0.00 %	0.19 %	0.00 %	99.81 %	
11.000	3.92	0.00 %	0.19 %	0.00 %	99.81 %	
12.000	3.92	0.00 %	0.19 %	0.00 %	99.81 %	

Carbonate and acidity

Carbonate 0.131 mM
Acidity error -0.266 mM

Other graphs

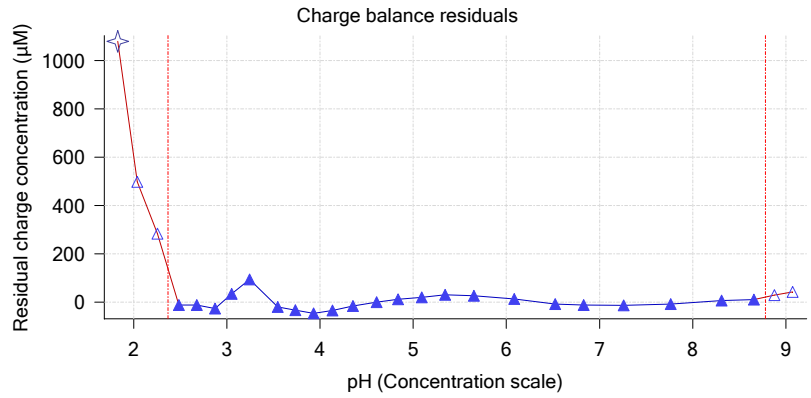


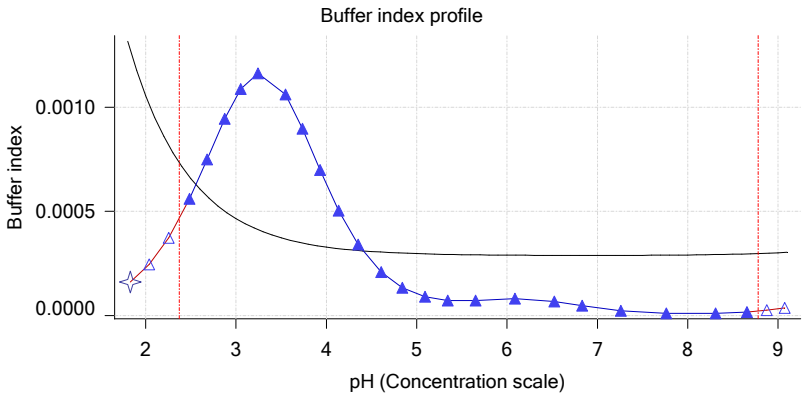


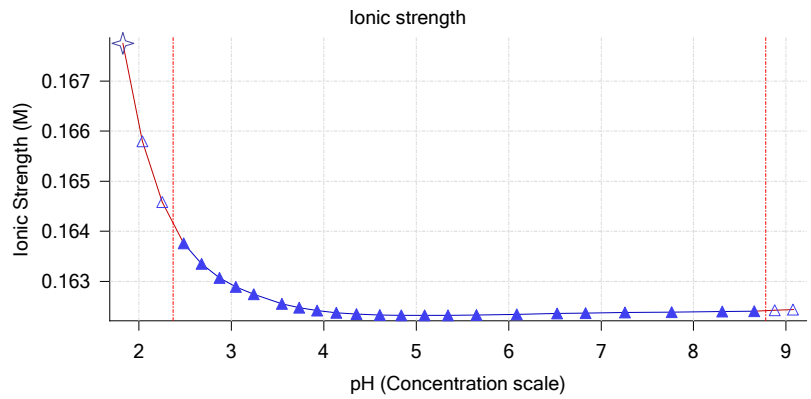
Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

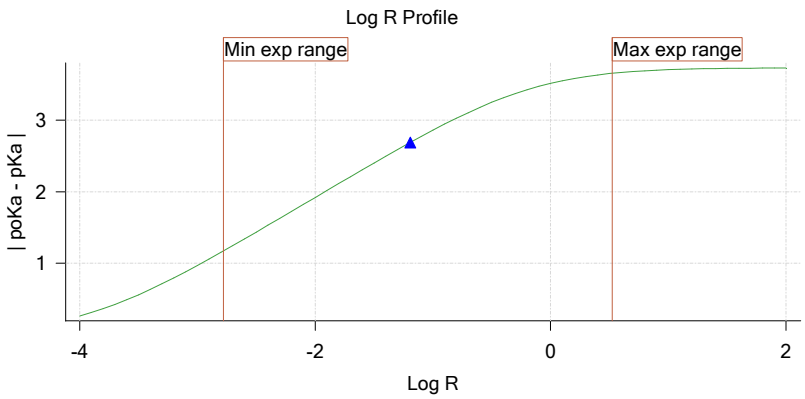
Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

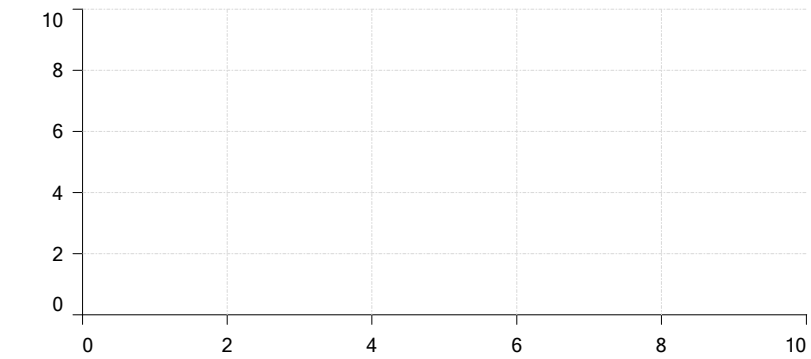
Other graphs (continued)

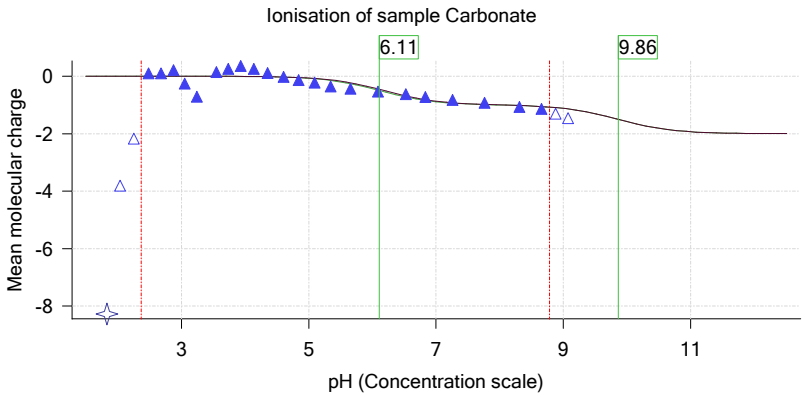












Sample name:	**M04_octanol**	Experiment start time:	**3/24/2018 4:11:23 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Dorothy Levorse**
Assay ID:	**18C-24004**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 3 of 3 18C-24004 Points 51 to 77

Overall results

RMSD	0.309
Average ionic strength	0.168 M
Average temperature	25.0°C
Partition ratio	0.2800 : 1
Analyte concentration range	2304.6 µM to 2362.2 µM
Total points considered	22 of 27

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.119	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
S	0.9972	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
jH	0.9	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
jOH	-0.3	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r

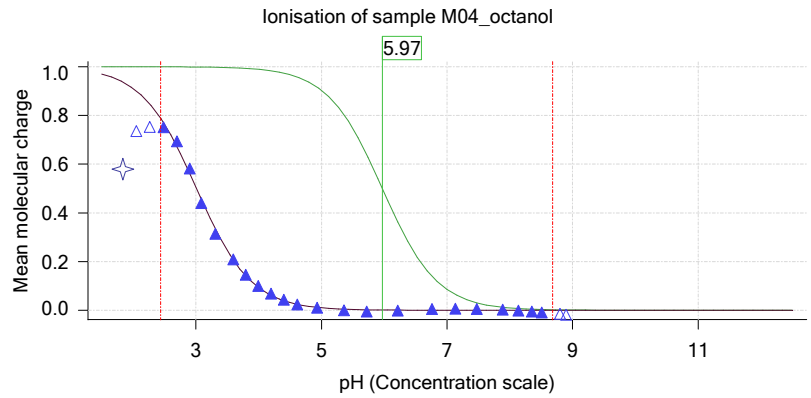
Titrants

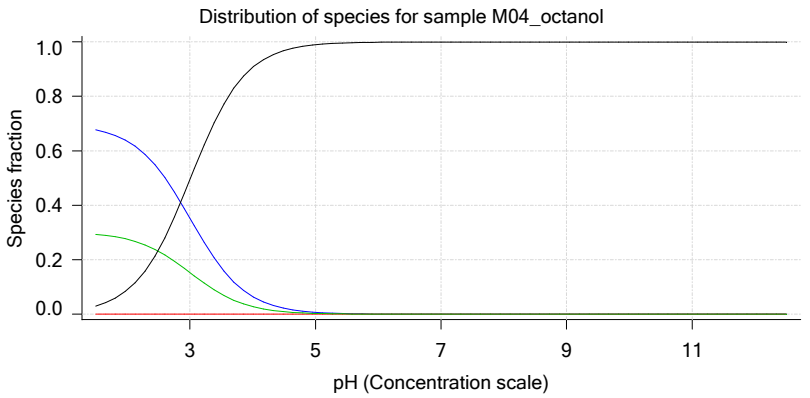
0.50 M HCl	0.997124	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
0.50 M KOH	1.003190	3/24/2018 4:11:23 AM	C:\Sirius_T3\KOH18C23.t3r

Sample

M04_octanol concentration factor	0.822
Base pKa 1	5.97
logP (XH +)	0.19
logP (neutral X)	3.67

Sample graphs

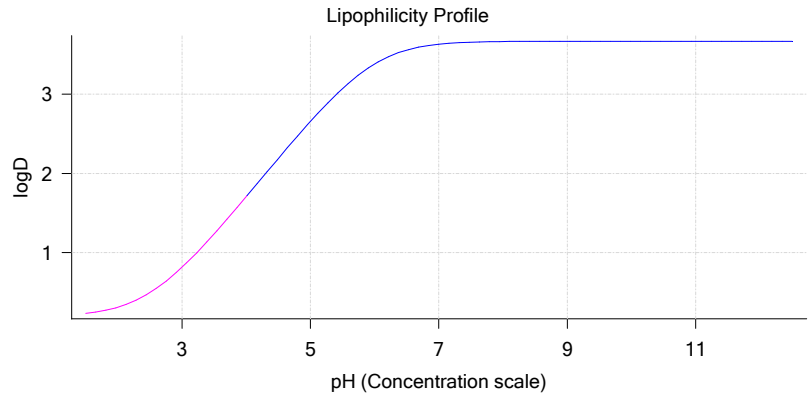




Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Sample graphs (continued)



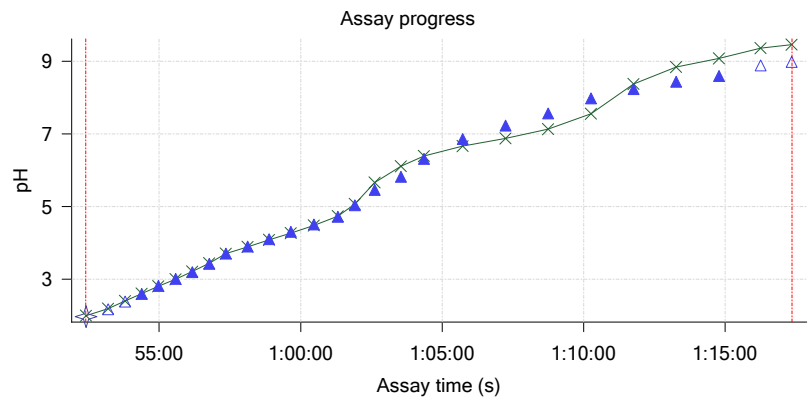
Sample logD and percent species

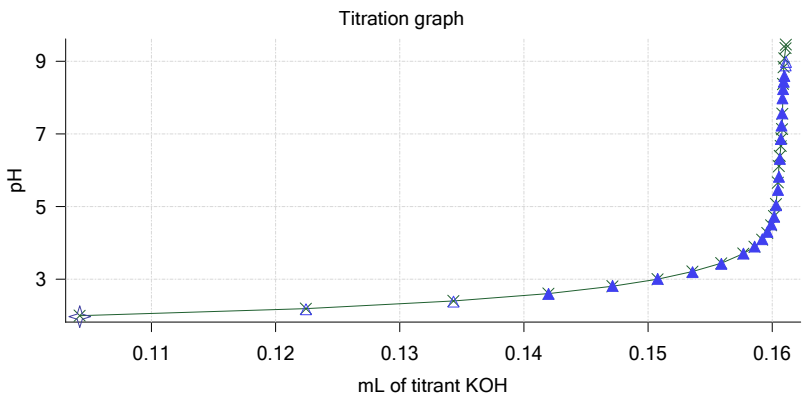
pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanol	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.20	69.08 %	0.00 %	29.96 %	0.97 %	
1.200	0.21	68.69 %	0.00 %	29.79 %	1.52 %	Stomach pH
2.000	0.31	63.55 %	0.01 %	27.56 %	8.88 %	
3.000	0.81	35.31 %	0.04 %	15.31 %	49.33 %	
4.000	1.71	6.49 %	0.07 %	2.81 %	90.63 %	
5.000	2.66	0.71 %	0.08 %	0.31 %	98.91 %	
6.000	3.38	0.07 %	0.08 %	0.03 %	99.82 %	
6.500	3.56	0.02 %	0.08 %	0.01 %	99.89 %	
7.000	3.63	0.01 %	0.08 %	0.00 %	99.91 %	
7.400	3.65	0.00 %	0.08 %	0.00 %	99.92 %	Blood pH
8.000	3.66	0.00 %	0.08 %	0.00 %	99.92 %	
9.000	3.67	0.00 %	0.08 %	0.00 %	99.92 %	
10.000	3.67	0.00 %	0.08 %	0.00 %	99.92 %	
11.000	3.67	0.00 %	0.08 %	0.00 %	99.92 %	
12.000	3.67	0.00 %	0.08 %	0.00 %	99.92 %	

Carbonate and acidity

Carbonate 0.118 mM
Acidity error -0.015 mM

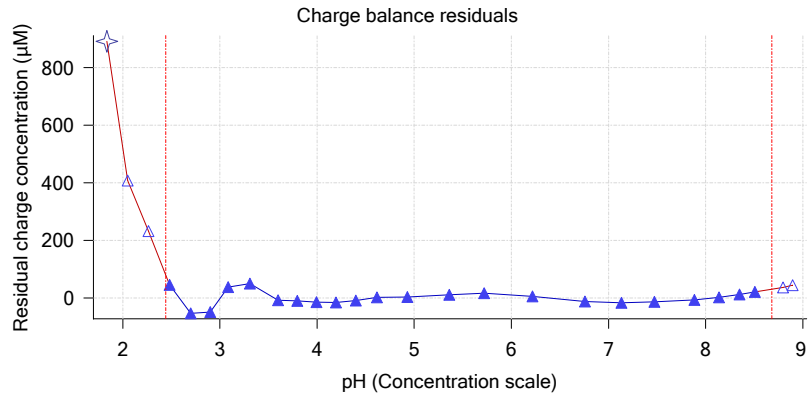
Other graphs

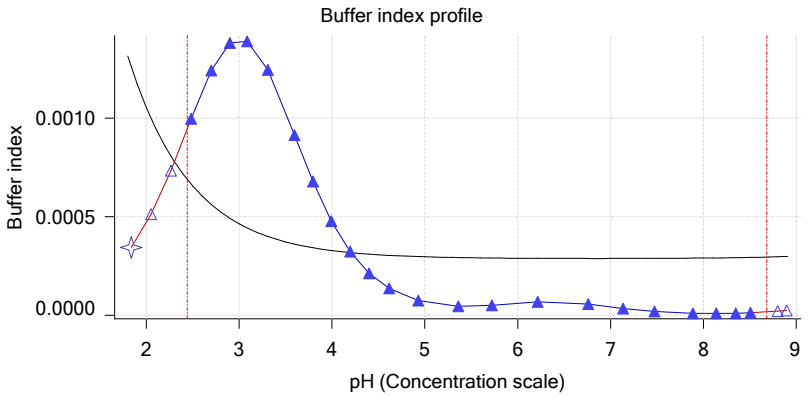


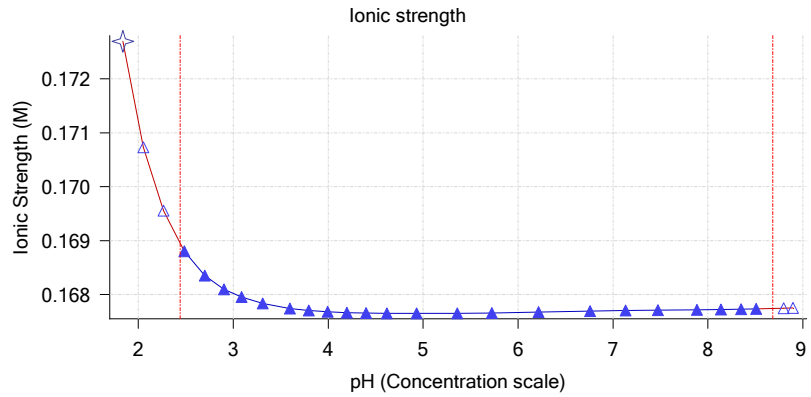


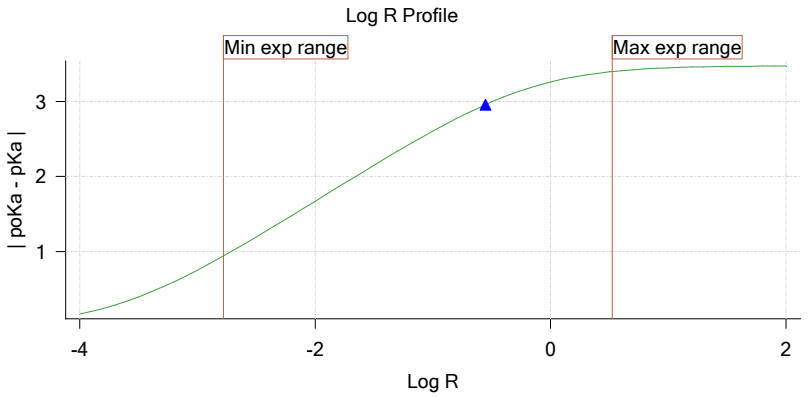
Sample name:	**M04_octanol**	Experiment start time:	**3/24/2018 4:11:23 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Dorothy Levorse**
Assay ID:	**18C-24004**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**		

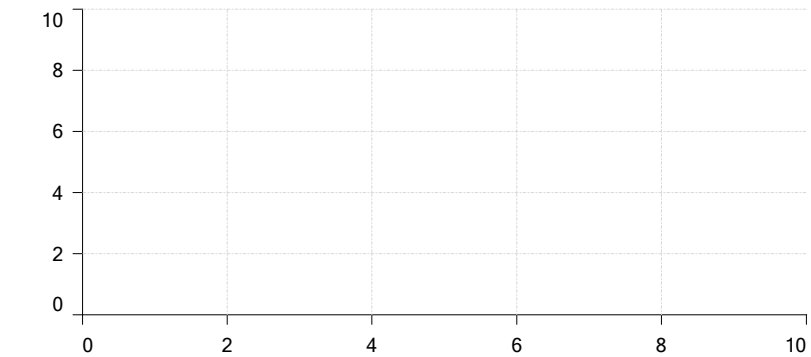
Other graphs (continued)

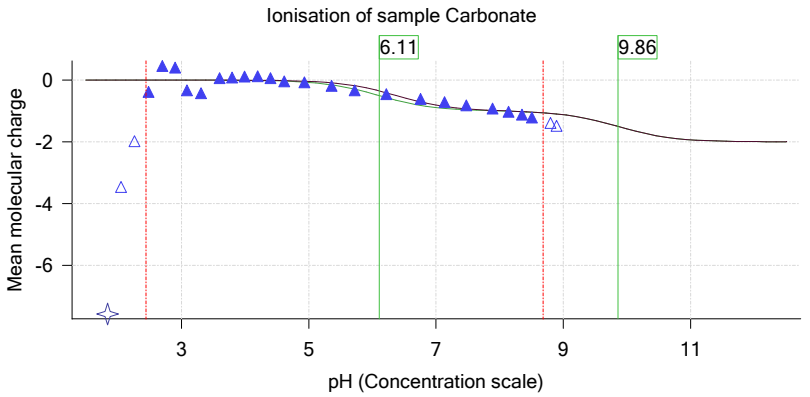












Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M04_octanol	3/9/2018 4:34:21 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001450 g	3/23/2018 5:00:45 PM	User entered value
Formula weight	269.73 g/mol	3/9/2018 4:34:21 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	269.73	3/9/2018 4:34:21 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	3/9/2018 4:34:21 PM	User entered value
Sample is a	Base	3/9/2018 4:34:21 PM	User entered value
pKa 1	5.97	3/9/2018 4:34:21 PM	User entered value
logp (XH +)	0.19	3/9/2018 4:34:33 PM	User entered value
logP (neutral X)	3.50	3/23/2018 2:32:46 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
5:00.3	Initial pH = 8.35									
7:60.0	Data point 1	1.50000 mL	0.05115 mL	0.00717 mL	0.03001 mL	2.013	-0.00513	0.25311	0.00050	10.0 s
8:46.2	Data point 2	1.50000 mL	0.05115 mL	0.02117 mL	0.03001 mL	2.222	0.00235	0.41042	0.00018	10.0 s
9:21.8	Data point 3	1.50000 mL	0.05115 mL	0.03024 mL	0.03001 mL	2.432	-0.00386	0.04058	0.00095	10.0 s
9:57.4	Data point 4	1.50000 mL	0.05115 mL	0.03589 mL	0.03001 mL	2.652	-0.00793	0.70535	0.00047	10.0 s
10:32.9	Data point 5	1.50000 mL	0.05115 mL	0.03937 mL	0.03001 mL	2.857	-0.00289	0.42030	0.00022	10.0 s
11:08.3	Data point 6	1.50000 mL	0.05115 mL	0.04165 mL	0.03001 mL	3.054	0.00006	0.00064	0.00011	10.0 s
11:43.9	Data point 7	1.50000 mL	0.05115 mL	0.04327 mL	0.03001 mL	3.257	-0.00042	0.04360	0.00010	10.5 s
12:19.7	Data point 8	1.50000 mL	0.05115 mL	0.04454 mL	0.03001 mL	3.464	-0.00064	0.06303	0.00013	10.0 s
12:55.2	Data point 9	1.50000 mL	0.05115 mL	0.04570 mL	0.03001 mL	3.661	-0.00672	0.71058	0.00039	10.5 s
13:31.1	Data point 10	1.50000 mL	0.05115 mL	0.04687 mL	0.03001 mL	3.861	-0.00883	0.75826	0.00050	10.0 s
14:06.6	Data point 11	1.50000 mL	0.05115 mL	0.04814 mL	0.03001 mL	4.103	-0.01310	0.89589	0.00068	10.5 s
14:47.7	Data point 12	1.50000 mL	0.05115 mL	0.04899 mL	0.03001 mL	4.289	-0.00937	0.84367	0.00050	10.5 s
15:23.5	Data point 13	1.50000 mL	0.05115 mL	0.04965 mL	0.03001 mL	4.508	-0.01463	0.74199	0.00084	11.0 s
15:59.9	Data point 14	1.50000 mL	0.05115 mL	0.05021 mL	0.03001 mL	4.755	-0.01555	0.81188	0.00085	13.0 s
16:38.2	Data point 15	1.50000 mL	0.05115 mL	0.05063 mL	0.03001 mL	5.109	-0.01643	0.85150	0.00088	17.0 s
17:20.6	Data point 16	1.50000 mL	0.05115 mL	0.05087 mL	0.03001 mL	5.521	-0.01966	0.95659	0.00099	21.0 s
18:12.1	Data point 17	1.50000 mL	0.05115 mL	0.05101 mL	0.03001 mL	5.806	-0.01764	0.91085	0.00091	29.5 s
19:12.2	Data point 18	1.50000 mL	0.05115 mL	0.05111 mL	0.03001 mL	6.280	-0.01792	0.93360	0.00092	45.5 s
20:28.4	Data point 19	1.50000 mL	0.05115 mL	0.05122 mL	0.03001 mL	7.844	-0.08873	0.99672	0.00439	Timed out at 59.5 s
21:58.9	Data point 20	1.50000 mL	0.05115 mL	0.05127 mL	0.03001 mL	8.410	-0.04014	0.97727	0.00201	Timed out at 59.5 s
23:29.4	Data point 21	1.50000 mL	0.05115 mL	0.05132 mL	0.03001 mL	8.719	-0.02194	0.97381	0.00110	Timed out at 59.5 s
25:05.0	Data point 22	1.50000 mL	0.05115 mL	0.05139 mL	0.03001 mL	8.993	-0.01950	0.95962	0.00098	34.5 s
26:05.0	Data point 23	1.50000 mL	0.05115 mL	0.05141 mL	0.03001 mL	9.001	-0.01921	0.96673	0.00097	42.0 s
27:41.8	Data point 24	1.50000 mL	0.10503 mL	0.05141 mL	0.11002 mL	1.955	-0.00341	0.14587	0.00044	10.0 s
28:28.0	Data point 25	1.50000 mL	0.10503 mL	0.06816 mL	0.11002 mL	2.160	0.00273	0.60068	0.00017	10.5 s
29:04.3	Data point 26	1.50000 mL	0.10503 mL	0.07947 mL	0.11002 mL	2.371	0.00238	0.28453	0.00022	10.0 s
29:39.9	Data point 27	1.50000 mL	0.10503 mL	0.08652 mL	0.11002 mL	2.601	0.00077	0.08864	0.00013	10.5 s
30:15.9	Data point 28	1.50000 mL	0.10503 mL	0.09087 mL	0.11002 mL	2.792	-0.01433	0.72766	0.00083	10.5 s
30:51.8	Data point 29	1.50000 mL	0.10503 mL	0.09393 mL	0.11002 mL	2.985	0.01516	0.73138	0.00088	10.0 s
31:27.3	Data point 30	1.50000 mL	0.10503 mL	0.09626 mL	0.11002 mL	3.161	-0.01511	0.64124	0.00093	11.0 s
32:14.1	Data point 31	1.50000 mL	0.10503 mL	0.09828 mL	0.11002 mL	3.353	-0.00936	0.31606	0.00082	10.0 s
32:49.5	Data point 32	1.50000 mL	0.10503 mL	0.10005 mL	0.11002 mL	3.657	-0.00287	0.78697	0.00016	10.5 s
33:30.6	Data point 33	1.50000 mL	0.10503 mL	0.10096 mL	0.11002 mL	3.844	-0.00635	0.80051	0.00035	10.0 s
34:06.0	Data point 34	1.50000 mL	0.10503 mL	0.10167 mL	0.11002 mL	4.038	-0.00491	0.70908	0.00029	10.0 s
34:41.4	Data point 35	1.50000 mL	0.10503 mL	0.10228 mL	0.11002 mL	4.243	-0.00496	0.59949	0.00032	10.0 s
35:16.8	Data point 36	1.50000 mL	0.10503 mL	0.10275 mL	0.11002 mL	4.459	-0.00596	0.57925	0.00039	10.5 s
35:52.7	Data point 37	1.50000 mL	0.10503 mL	0.10310 mL	0.11002 mL	4.712	0.00092	0.00227	0.00095	10.5 s

Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
36:28.6	Data point 38	1.50000 mL	0.10503 mL	0.10332 mL	0.11002 mL	4.945	-0.00605	0.33921	0.00051	11.0 s
37:05.0	Data point 39	1.50000 mL	0.10503 mL	0.10346 mL	0.11002 mL	5.195	-0.01462	0.70458	0.00086	12.0 s
37:47.6	Data point 40	1.50000 mL	0.10503 mL	0.10358 mL	0.11002 mL	5.448	-0.00465	0.09101	0.00076	13.0 s
38:31.1	Data point 41	1.50000 mL	0.10503 mL	0.10365 mL	0.11002 mL	5.756	-0.01450	0.74805	0.00083	15.5 s
39:17.2	Data point 42	1.50000 mL	0.10503 mL	0.10372 mL	0.11002 mL	6.188	-0.01751	0.88071	0.00092	38.0 s
40:25.8	Data point 43	1.50000 mL	0.10503 mL	0.10376 mL	0.11002 mL	6.624	-0.01828	0.88671	0.00096	59.5 s
41:50.7	Data point 44	1.50000 mL	0.10503 mL	0.10381 mL	0.11002 mL	6.931	-0.02021	0.98765	0.00100	Timed out at 59.5 s
43:21.2	Data point 45	1.50000 mL	0.10503 mL	0.10386 mL	0.11002 mL	7.358	-0.05882	0.99495	0.00291	Timed out at 59.5 s
44:51.6	Data point 46	1.50000 mL	0.10503 mL	0.10390 mL	0.11002 mL	7.860	-0.06638	0.98979	0.00330	Timed out at 59.5 s
46:27.2	Data point 47	1.50000 mL	0.10503 mL	0.10398 mL	0.11002 mL	8.405	-0.03574	0.99078	0.00177	Timed out at 59.5 s
47:57.6	Data point 48	1.50000 mL	0.10503 mL	0.10402 mL	0.11002 mL	8.751	-0.01947	0.94555	0.00099	58.0 s
49:26.2	Data point 49	1.50000 mL	0.10503 mL	0.10412 mL	0.11002 mL	8.970	-0.01588	0.97546	0.00079	42.0 s
50:38.7	Data point 50	1.50000 mL	0.10503 mL	0.10421 mL	0.11002 mL	9.167	-0.01890	0.92626	0.00097	28.5 s
52:25.2	Data point 51	1.50000 mL	0.16148 mL	0.10421 mL	0.51002 mL	1.964	-0.00413	0.66600	0.00025	10.5 s
53:11.9	Data point 52	1.50000 mL	0.16148 mL	0.12244 mL	0.51002 mL	2.173	0.00880	0.67097	0.00053	10.0 s
53:47.6	Data point 53	1.50000 mL	0.16148 mL	0.13434 mL	0.51002 mL	2.382	0.01052	0.53800	0.00071	10.0 s
54:23.2	Data point 54	1.50000 mL	0.16148 mL	0.14198 mL	0.51002 mL	2.597	-0.00151	0.05969	0.00031	10.0 s
54:58.7	Data point 55	1.50000 mL	0.16148 mL	0.14713 mL	0.51002 mL	2.812	-0.00306	0.69301	0.00018	10.5 s
55:34.7	Data point 56	1.50000 mL	0.16148 mL	0.15078 mL	0.51002 mL	3.013	-0.00746	0.20419	0.00082	10.0 s
56:10.2	Data point 57	1.50000 mL	0.16148 mL	0.15360 mL	0.51002 mL	3.197	0.00123	0.02683	0.00037	10.5 s
56:46.2	Data point 58	1.50000 mL	0.16148 mL	0.15590 mL	0.51002 mL	3.420	-0.00821	0.19314	0.00092	10.0 s
57:21.7	Data point 59	1.50000 mL	0.16148 mL	0.15769 mL	0.51002 mL	3.707	0.00459	0.14616	0.00059	10.0 s
58:07.4	Data point 60	1.50000 mL	0.16148 mL	0.15858 mL	0.51002 mL	3.903	-0.00128	0.00501	0.00089	10.0 s
58:53.1	Data point 61	1.50000 mL	0.16148 mL	0.15920 mL	0.51002 mL	4.102	-0.00123	0.00430	0.00093	10.0 s
59:38.9	Data point 62	1.50000 mL	0.16148 mL	0.15962 mL	0.51002 mL	4.303	-0.01215	0.38768	0.00096	13.5 s
1:00:28.1	Data point 63	1.50000 mL	0.16148 mL	0.15993 mL	0.51002 mL	4.507	-0.00113	0.00611	0.00072	10.0 s
1:01:18.9	Data point 64	1.50000 mL	0.16148 mL	0.16016 mL	0.51002 mL	4.723	0.00118	0.00902	0.00061	10.5 s
1:01:54.8	Data point 65	1.50000 mL	0.16148 mL	0.16033 mL	0.51002 mL	5.036	-0.01870	0.92089	0.00096	11.5 s
1:02:36.9	Data point 66	1.50000 mL	0.16148 mL	0.16047 mL	0.51002 mL	5.464	-0.01865	0.92187	0.00096	25.0 s
1:03:32.5	Data point 67	1.50000 mL	0.16148 mL	0.16056 mL	0.51002 mL	5.825	-0.01533	0.67266	0.00092	18.5 s
1:04:21.6	Data point 68	1.50000 mL	0.16148 mL	0.16063 mL	0.51002 mL	6.318	-0.01905	0.96692	0.00096	51.5 s
1:05:43.7	Data point 69	1.50000 mL	0.16148 mL	0.16070 mL	0.51002 mL	6.858	-0.05249	0.96745	0.00264	Timed out at 59.5 s
1:07:14.2	Data point 70	1.50000 mL	0.16148 mL	0.16075 mL	0.51002 mL	7.233	-0.05610	0.97962	0.00280	Timed out at 59.5 s
1:08:44.7	Data point 71	1.50000 mL	0.16148 mL	0.16079 mL	0.51002 mL	7.571	-0.05662	0.99069	0.00281	Timed out at 59.5 s
1:10:15.2	Data point 72	1.50000 mL	0.16148 mL	0.16084 mL	0.51002 mL	7.982	-0.05547	0.99203	0.00275	Timed out at 59.5 s
1:11:45.7	Data point 73	1.50000 mL	0.16148 mL	0.16089 mL	0.51002 mL	8.235	-0.05197	0.96437	0.00261	Timed out at 59.5 s
1:13:16.2	Data point 74	1.50000 mL	0.16148 mL	0.16094 mL	0.51002 mL	8.444	-0.02913	0.98679	0.00145	Timed out at 59.5 s
1:14:46.7	Data point 75	1.50000 mL	0.16148 mL	0.16098 mL	0.51002 mL	8.602	-0.01977	0.98733	0.00098	47.0 s
1:16:14.7	Data point 76	1.50000 mL	0.16148 mL	0.16108 mL	0.51002 mL	8.892	-0.01379	0.56644	0.00091	35.5 s
1:17:20.7	Data point 77	1.50000 mL	0.16148 mL	0.16112 mL	0.51002 mL	8.988	-0.01977	0.96525	0.00099	28.5 s
1:17:58.3	Assay volumes	1.50000 mL	0.16148 mL	0.16112 mL	0.51002 mL					

Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.030 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	60 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.080 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.400 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.119	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
Four-Plus S	0.9972	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
Four-Plus jH	0.9	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
Four-Plus jOH	-0.3	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r
Base concentration factor	1.003	3/24/2018 4:11:23 AM	C:\Sirius_T3\KOH18C23.t3r
Acid concentration factor	0.997	3/24/2018 4:11:23 AM	C:\Sirius_T3\HCl18C23.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	3/16/2018 11:09:18 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	03-16-2018	3/16/2018 10:56:23 AM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	3/22/2018	3/23/2018 9:34:17 AM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	02-08-2018	3/6/2018 10:28:59 AM
Port B	Cyclohexane	11-01-17	2/27/2018 11:37:57 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 11:18:04 AM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM

Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 10:59:35 AM
Titrator		T3TM1200161	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 3:01:00 PM
E0 calibration	+4.67 mV		3/24/2018 4:11:51 AM
Filling solution	3M KCl	KCL097	3/23/2018 9:29:07 AM
Liquids			
Wash 1	50% IPA:50% Water		3/23/2018 9:29:12 AM
Wash 2	0.5% Trition X-100 in H20		3/23/2018 9:29:15 AM
Buffer position 1	pH7 Wash		3/23/2018 9:29:19 AM
Buffer position 2	pH 7		3/23/2018 9:29:21 AM
Storage position			3/23/2018 9:30:23 AM
Wash water	7.6e+003 mL	03-12-2018	3/12/2018 9:25:04 AM
Waste	2.6e+003 mL		3/12/2018 9:24:49 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		074811	11/23/2010 12:22:28 PM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	162:53:01		11/23/2010 12:22:28 PM
Calibrated on	2/27/2018 11:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24004**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24004_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 4:11:23 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00